

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **6**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|--------|----------|----------|----------|--------|
| Sc | 7151(1) | 1417(1) | 8442(1) | 23(1) |
| Si | 9380(1) | 655(1) | 8041(1) | 39(1) |
| C(1) | 8803(2) | 2200(2) | 8244(1) | 28(1) |
| C(2) | 8175(2) | 2765(2) | 7682(1) | 25(1) |
| C(3) | 7548(2) | 3646(2) | 7995(1) | 30(1) |
| C(4) | 7775(2) | 3608(3) | 8766(2) | 38(1) |
| C(5) | 8526(2) | 2738(2) | 8927(1) | 33(1) |
| C(6) | 8245(2) | -297(2) | 8104(1) | 32(1) |
| C(7) | 7397(2) | -377(2) | 7609(1) | 35(1) |
| C(8) | 6594(2) | -754(2) | 8015(1) | 38(1) |
| C(9) | 6900(2) | -926(2) | 8767(1) | 31(1) |
| C(10) | 7901(2) | -626(2) | 8817(1) | 32(1) |
| C(11) | 10333(2) | 71(4) | 8737(2) | 74(1) |
| C(12) | 9935(2) | 703(3) | 7120(2) | 56(1) |
| C(13) | 5970(2) | 1799(4) | 9421(2) | 57(1) |
| C(14A) | 5640(4) | 2449(9) | 8822(5) | 66(3) |
| C(14B) | 5452(6) | 1515(13) | 8786(6) | 53(4) |
| C(15) | 5439(2) | 2014(4) | 8110(3) | 63(1) |
| C(30) | 6861(2) | 4550(3) | 7578(2) | 47(1) |
| C(31) | 7308(2) | 5859(3) | 7549(2) | 68(1) |
| C(32) | 6580(2) | 4099(3) | 6797(2) | 62(1) |
| C(50) | 8998(2) | 2465(3) | 9689(2) | 52(1) |
| C(51) | 10009(3) | 3033(6) | 9771(2) | 150(3) |
| C(52) | 8375(4) | 2851(4) | 10316(2) | 83(1) |
| C(70) | 7382(3) | -170(3) | 6774(1) | 48(1) |
| C(71) | 7899(5) | -1281(3) | 6411(2) | 113(3) |
| C(72) | 6375(3) | 34(4) | 6427(2) | 89(2) |
| C(90) | 6305(2) | -1485(3) | 9370(1) | 35(1) |
| C(91) | 6136(3) | -2888(3) | 9238(2) | 63(1) |
| C(92) | 6778(2) | -1273(3) | 10138(1) | 48(1) |

Table 4. Bond lengths [Å] and angles [deg] for **6**.

| | |
|---------------|-----------|
| Sc-X(1A) | 2.1875(5) |
| Sc-X(1B) | 2.1894(6) |
| Sc-Pln(A) | 2.184(2) |
| Sc-Pln(B) | 2.184(2) |
| Sc-C(14B) | 2.436(7) |
| Sc-C(6) | 2.450(2) |
| Sc-C(1) | 2.450(2) |
| Sc-C(7) | 2.457(2) |
| Sc-C(14A) | 2.465(5) |
| Sc-C(2) | 2.465(2) |
| Sc-C(15) | 2.469(3) |
| Sc-C(5) | 2.469(2) |
| Sc-C(10) | 2.476(3) |
| Sc-C(13) | 2.487(3) |
| Si-C(1) | 1.862(3) |
| Si-C(12) | 1.864(3) |
| Si-C(6) | 1.859(3) |
| Si-C(11) | 1.869(3) |
| C(1)-C(2) | 1.428(3) |
| C(1)-C(5) | 1.428(3) |
| C(2)-C(3) | 1.406(3) |
| C(2)-H(2) | 0.96(2) |
| C(3)-C(4) | 1.412(4) |
| C(3)-C(30) | 1.515(4) |
| C(4)-C(5) | 1.400(4) |
| C(4)-H(4) | 0.87(3) |
| C(5)-C(50) | 1.518(4) |
| C(6)-C(7) | 1.429(4) |
| C(6)-C(10) | 1.436(3) |
| C(7)-C(8) | 1.408(4) |
| C(7)-C(70) | 1.523(3) |
| C(8)-C(9) | 1.412(3) |
| C(8)-H(8) | 0.91(3) |
| C(9)-C(10) | 1.403(4) |
| C(9)-C(90) | 1.513(3) |
| C(10)-H(10) | 0.94(2) |
| C(11)-H(11A) | 0.90(2) |
| C(11)-H(11B) | 0.90(2) |
| C(11)-H(11C) | 0.90(2) |
| C(12)-H(12A) | 0.95(2) |
| C(12)-H(12B) | 0.95(2) |
| C(12)-H(12C) | 0.95(2) |
| C(13)-C(14A) | 1.340(8) |
| C(13)-C(14B) | 1.349(11) |
| C(13)-H(13A) | 0.961(4) |
| C(13)-H(13B) | 0.958(4) |
| C(13)-H(13C) | 0.963(4) |
| C(13)-H(13D) | 0.958(4) |
| C(14A)-C(15) | 1.381(9) |
| C(14A)-H(14A) | 0.906(10) |
| C(14A)-H(13C) | 1.431(9) |
| C(14A)-H(15C) | 1.483(8) |
| C(14B)-C(15) | 1.331(12) |
| C(14B)-H(14B) | 0.868(13) |
| C(30)-C(31) | 1.518(4) |
| C(30)-C(32) | 1.519(4) |
| C(30)-H(30) | 0.98(2) |
| C(31)-H(31A) | 0.99(2) |
| C(31)-H(31B) | 0.99(2) |
| C(31)-H(31C) | 0.99(2) |
| C(32)-H(32A) | 0.97(2) |
| C(32)-H(32B) | 0.97(2) |

| | |
|--------------|-----------|
| C(32)-H(32C) | 0.97(2) |
| C(50)-C(52) | 1.507(4) |
| C(50)-C(51) | 1.509(4) |
| C(50)-H(50) | 0.99(2) |
| C(51)-H(51A) | 1.03(2) |
| C(51)-H(51B) | 1.03(2) |
| C(51)-H(51C) | 1.03(2) |
| C(52)-H(52A) | 0.95(2) |
| C(52)-H(52B) | 0.95(2) |
| C(52)-H(52C) | 0.95(2) |
| C(70)-C(72) | 1.499(5) |
| C(70)-C(71) | 1.537(5) |
| C(70)-H(70) | 0.97(2) |
| C(71)-H(71A) | 0.89(2) |
| C(71)-H(71B) | 0.89(2) |
| C(71)-H(71C) | 0.89(2) |
| C(72)-H(72A) | 0.95(2) |
| C(72)-H(72B) | 0.95(2) |
| C(72)-H(72C) | 0.95(2) |
| C(90)-C(92) | 1.518(4) |
| C(90)-C(91) | 1.522(4) |
| C(90)-H(90) | 0.91(2) |
| C(91)-H(91A) | 0.95(2) |
| C(91)-H(91B) | 0.95(2) |
| C(91)-H(91C) | 0.95(2) |
| C(92)-H(92A) | 0.983(13) |
| C(92)-H(92B) | 0.983(13) |
| C(92)-H(92C) | 0.983(13) |

| | |
|------------------|------------|
| X(1A)-Sc-X(1B) | 128.49(2) |
| Pln(A)-Sc-Pln(B) | 121.48(9) |
| C(14B)-Sc-C(6) | 134.2(3) |
| C(14B)-Sc-C(1) | 157.0(3) |
| C(6)-Sc-C(1) | 68.66(9) |
| C(14B)-Sc-C(7) | 110.5(3) |
| C(6)-Sc-C(7) | 33.87(9) |
| C(1)-Sc-C(7) | 90.99(9) |
| C(6)-Sc-C(14A) | 158.3(2) |
| C(1)-Sc-C(14A) | 133.0(2) |
| C(7)-Sc-C(14A) | 131.0(2) |
| C(14B)-Sc-C(2) | 133.8(3) |
| C(6)-Sc-C(2) | 85.45(8) |
| C(1)-Sc-C(2) | 33.78(8) |
| C(7)-Sc-C(2) | 90.52(8) |
| C(14A)-Sc-C(2) | 113.9(2) |
| C(14B)-Sc-C(15) | 31.5(3) |
| C(6)-Sc-C(15) | 135.47(14) |
| C(1)-Sc-C(15) | 138.37(10) |
| C(7)-Sc-C(15) | 101.97(14) |
| C(14A)-Sc-C(15) | 32.5(2) |
| C(2)-Sc-C(15) | 105.91(10) |
| C(14B)-Sc-C(5) | 127.1(3) |
| C(6)-Sc-C(5) | 92.62(9) |
| C(1)-Sc-C(5) | 33.75(8) |
| C(7)-Sc-C(5) | 122.05(9) |
| C(14A)-Sc-C(5) | 106.4(2) |
| C(2)-Sc-C(5) | 54.94(8) |
| C(15)-Sc-C(5) | 129.50(12) |
| C(14B)-Sc-C(10) | 110.7(3) |
| C(6)-Sc-C(10) | 33.89(8) |
| C(1)-Sc-C(10) | 87.95(9) |
| C(7)-Sc-C(10) | 54.75(8) |
| C(14A)-Sc-C(10) | 130.8(2) |
| C(2)-Sc-C(10) | 114.87(8) |
| C(15)-Sc-C(10) | 131.68(11) |
| C(5)-Sc-C(10) | 95.83(9) |

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|-----------------|------------|
| C(14B)-Sc-C(13) | 31.8(3) |
| C(6)-Sc-C(13) | 136.39(10) |
| C(1)-Sc-C(13) | 133.25(12) |
| C(7)-Sc-C(13) | 132.42(11) |
| C(14A)-Sc-C(13) | 31.4(2) |
| C(2)-Sc-C(13) | 135.11(10) |
| C(15)-Sc-C(13) | 59.28(14) |
| C(5)-Sc-C(13) | 99.51(11) |
| C(10)-Sc-C(13) | 102.86(10) |
| C(1)-Si-C(12) | 110.26(13) |
| C(1)-Si-C(6) | 95.92(10) |
| C(12)-Si-C(6) | 116.6(2) |
| C(1)-Si-C(11) | 116.5(2) |
| C(12)-Si-C(11) | 107.93(14) |
| C(6)-Si-C(11) | 109.5(2) |
| C(1)-Si-Sc | 47.99(7) |
| C(12)-Si-Sc | 128.09(10) |
| C(6)-Si-Sc | 47.98(7) |
| C(11)-Si-Sc | 123.98(11) |
| C(2)-C(1)-C(5) | 105.7(2) |
| C(2)-C(1)-Si | 118.4(2) |
| C(5)-C(1)-Si | 130.9(2) |
| C(2)-C(1)-Sc | 73.71(13) |
| C(5)-C(1)-Sc | 73.89(13) |
| Si-C(1)-Sc | 97.63(10) |
| C(3)-C(2)-C(1) | 110.5(2) |
| C(3)-C(2)-Sc | 77.68(14) |
| C(1)-C(2)-Sc | 72.52(13) |
| C(3)-C(2)-H(2) | 125.8(14) |
| C(1)-C(2)-H(2) | 123.7(14) |
| Sc-C(2)-H(2) | 117.8(14) |
| C(2)-C(3)-C(4) | 105.7(2) |
| C(2)-C(3)-C(30) | 126.5(2) |
| C(4)-C(3)-C(30) | 127.5(2) |
| C(2)-C(3)-Sc | 69.94(13) |
| C(4)-C(3)-Sc | 72.7(2) |
| C(30)-C(3)-Sc | 127.1(2) |
| C(5)-C(4)-C(3) | 110.2(2) |
| C(5)-C(4)-Sc | 71.3(2) |
| C(3)-C(4)-Sc | 75.1(2) |
| C(5)-C(4)-H(4) | 126(2) |
| C(3)-C(4)-H(4) | 124(2) |
| Sc-C(4)-H(4) | 123(2) |
| C(4)-C(5)-C(1) | 107.9(2) |
| C(4)-C(5)-C(50) | 125.9(2) |
| C(1)-C(5)-C(50) | 126.1(3) |
| C(4)-C(5)-Sc | 76.3(2) |
| C(1)-C(5)-Sc | 72.37(13) |
| C(50)-C(5)-Sc | 119.6(2) |
| C(7)-C(6)-C(10) | 104.7(2) |
| C(7)-C(6)-Si | 130.3(2) |
| C(10)-C(6)-Si | 119.9(2) |
| C(7)-C(6)-Sc | 73.37(14) |
| C(10)-C(6)-Sc | 74.06(14) |
| Si-C(6)-Sc | 97.71(11) |
| C(8)-C(7)-C(6) | 108.7(2) |
| C(8)-C(7)-C(70) | 125.7(3) |
| C(6)-C(7)-C(70) | 125.5(3) |
| C(8)-C(7)-Sc | 76.6(2) |
| C(6)-C(7)-Sc | 72.77(13) |
| C(70)-C(7)-Sc | 119.9(2) |
| C(9)-C(8)-C(7) | 109.6(2) |
| C(9)-C(8)-Sc | 75.8(2) |
| C(7)-C(8)-Sc | 70.69(14) |
| C(9)-C(8)-H(8) | 126(2) |
| C(7)-C(8)-H(8) | 124(2) |

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|----------------------|------------|
| Sc-C(8)-H(8) | 121(2) |
| C(10)-C(9)-C(8) | 105.9(2) |
| C(10)-C(9)-C(90) | 126.9(2) |
| C(8)-C(9)-C(90) | 126.7(2) |
| C(10)-C(9)-Sc | 69.87(14) |
| C(8)-C(9)-Sc | 72.16(14) |
| C(90)-C(9)-Sc | 128.6(2) |
| C(9)-C(10)-C(6) | 111.1(2) |
| C(9)-C(10)-Sc | 77.97(14) |
| C(6)-C(10)-Sc | 72.05(14) |
| C(9)-C(10)-H(10) | 126(2) |
| C(6)-C(10)-H(10) | 123(2) |
| Sc-C(10)-H(10) | 118(2) |
| Si-C(11)-H(11A) | 109.47(10) |
| Si-C(11)-H(11B) | 109.47(14) |
| H(11A)-C(11)-H(11B) | 109.5 |
| Si-C(11)-H(11C) | 109.47(14) |
| H(11A)-C(11)-H(11C) | 109.5 |
| H(11B)-C(11)-H(11C) | 109.5 |
| Si-C(12)-H(12A) | 109.47(10) |
| Si-C(12)-H(12B) | 109.47(10) |
| H(12A)-C(12)-H(12B) | 109.5 |
| Si-C(12)-H(12C) | 109.47(12) |
| H(12A)-C(12)-H(12C) | 109.5 |
| H(12B)-C(12)-H(12C) | 109.5 |
| C(14A)-C(13)-Sc | 73.4(2) |
| C(14B)-C(13)-Sc | 72.1(3) |
| C(14A)-C(13)-H(13A) | 115.1(5) |
| Sc-C(13)-H(13A) | 116.2(2) |
| C(14A)-C(13)-H(13B) | 117.0(5) |
| Sc-C(13)-H(13B) | 116.4(3) |
| H(13A)-C(13)-H(13B) | 113.2(4) |
| C(14B)-C(13)-H(13C) | 115.4(6) |
| Sc-C(13)-H(13C) | 116.3(2) |
| C(14B)-C(13)-H(13D) | 117.4(7) |
| Sc-C(13)-H(13D) | 116.5(2) |
| H(13C)-C(13)-H(13D) | 113.2(4) |
| C(13)-C(14A)-C(15) | 128.5(7) |
| C(13)-C(14A)-Sc | 75.2(3) |
| C(15)-C(14A)-Sc | 73.9(3) |
| C(13)-C(14A)-H(14A) | 106.2(8) |
| C(15)-C(14A)-H(14A) | 121.6(7) |
| Sc-C(14A)-H(14A) | 106.4(4) |
| C(13)-C(14A)-H(13C) | 40.5(3) |
| C(15)-C(14A)-H(13C) | 168.9(7) |
| Sc-C(14A)-H(13C) | 99.0(3) |
| C(13)-C(14A)-H(15C) | 160.8(6) |
| C(15)-C(14A)-H(15C) | 35.5(3) |
| Sc-C(14A)-H(15C) | 87.6(3) |
| H(13C)-C(14A)-H(15C) | 154.7(7) |
| C(15)-C(14B)-C(13) | 132.3(10) |
| C(15)-C(14B)-Sc | 75.6(4) |
| C(13)-C(14B)-Sc | 76.2(4) |
| C(15)-C(14B)-H(13B) | 171.6(10) |
| C(13)-C(14B)-H(13B) | 39.4(4) |
| Sc-C(14B)-H(13B) | 98.9(4) |
| C(15)-C(14B)-H(15A) | 41.6(4) |
| C(13)-C(14B)-H(15A) | 161.4(6) |
| Sc-C(14B)-H(15A) | 85.4(4) |
| H(13B)-C(14B)-H(15A) | 145.4(10) |
| C(15)-C(14B)-H(14B) | 117.8(12) |
| C(13)-C(14B)-H(14B) | 108.2(11) |
| Sc-C(14B)-H(14B) | 112.3(7) |
| C(14B)-C(15)-Sc | 72.9(3) |
| C(14A)-C(15)-Sc | 73.6(2) |
| C(14A)-C(15)-H(15B) | 132.3(6) |

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|---------------------|-----------|
| Sc-C(15)-H(15B) | 121.7(3) |
| C(14A)-C(15)-H(15A) | 121.6(5) |
| Sc-C(15)-H(15A) | 95.1(2) |
| H(15B)-C(15)-H(15A) | 102.9(5) |
| C(14B)-C(15)-H(15C) | 122.1(8) |
| Sc-C(15)-H(15C) | 104.7(2) |
| C(14B)-C(15)-H(15D) | 116.8(7) |
| Sc-C(15)-H(15D) | 115.8(3) |
| H(15C)-C(15)-H(15D) | 115.5(4) |
| C(31)-C(30)-C(32) | 109.8(3) |
| C(31)-C(30)-C(3) | 110.8(3) |
| C(32)-C(30)-C(3) | 112.6(2) |
| C(31)-C(30)-H(30) | 107.7(14) |
| C(32)-C(30)-H(30) | 107(2) |
| C(3)-C(30)-H(30) | 108.8(14) |
| C(30)-C(31)-H(31A) | 109.5(2) |
| C(30)-C(31)-H(31B) | 109.5(2) |
| H(31A)-C(31)-H(31B) | 109.5 |
| C(30)-C(31)-H(31C) | 109.5(2) |
| H(31A)-C(31)-H(31C) | 109.5 |
| H(31B)-C(31)-H(31C) | 109.5 |
| C(30)-C(32)-H(32A) | 109.5(2) |
| C(30)-C(32)-H(32B) | 109.5(2) |
| H(32A)-C(32)-H(32B) | 109.5 |
| C(30)-C(32)-H(32C) | 109.5(2) |
| H(32A)-C(32)-H(32C) | 109.5 |
| H(32B)-C(32)-H(32C) | 109.5 |
| C(52)-C(50)-C(5) | 113.5(3) |
| C(52)-C(50)-C(51) | 111.6(4) |
| C(5)-C(50)-C(51) | 110.9(3) |
| C(52)-C(50)-H(50) | 107(2) |
| C(5)-C(50)-H(50) | 111(2) |
| C(51)-C(50)-H(50) | 103(2) |
| C(50)-C(51)-H(51A) | 109.5(2) |
| C(50)-C(51)-H(51B) | 109.5(3) |
| H(51A)-C(51)-H(51B) | 109.5 |
| C(50)-C(51)-H(51C) | 109.5(3) |
| H(51A)-C(51)-H(51C) | 109.5 |
| H(51B)-C(51)-H(51C) | 109.5 |
| C(50)-C(52)-H(52A) | 109.5(2) |
| C(50)-C(52)-H(52B) | 109.5(2) |
| H(52A)-C(52)-H(52B) | 109.5 |
| C(50)-C(52)-H(52C) | 109.5(2) |
| H(52A)-C(52)-H(52C) | 109.5 |
| H(52B)-C(52)-H(52C) | 109.5 |
| C(72)-C(70)-C(7) | 113.7(3) |
| C(72)-C(70)-C(71) | 111.4(4) |
| C(7)-C(70)-C(71) | 109.2(3) |
| C(72)-C(70)-H(70) | 107.8(13) |
| C(7)-C(70)-H(70) | 108.6(13) |
| C(71)-C(70)-H(70) | 105.8(13) |
| C(70)-C(71)-H(71A) | 109.5(2) |
| C(70)-C(71)-H(71B) | 109.5(3) |
| H(71A)-C(71)-H(71B) | 109.5 |
| C(70)-C(71)-H(71C) | 109.5(2) |
| H(71A)-C(71)-H(71C) | 109.5 |
| H(71B)-C(71)-H(71C) | 109.5 |
| C(70)-C(72)-H(72A) | 109.5(2) |
| C(70)-C(72)-H(72B) | 109.5(2) |
| H(72A)-C(72)-H(72B) | 109.5 |
| C(70)-C(72)-H(72C) | 109.5(2) |
| H(72A)-C(72)-H(72C) | 109.5 |
| H(72B)-C(72)-H(72C) | 109.5 |
| C(92)-C(90)-C(9) | 112.3(2) |
| C(92)-C(90)-C(91) | 110.0(2) |
| C(9)-C(90)-C(91) | 110.7(2) |

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|---------------------|------------|
| C(92)-C(90)-H(90) | 107(2) |
| C(9)-C(90)-H(90) | 108(2) |
| C(91)-C(90)-H(90) | 110(2) |
| C(90)-C(91)-H(91A) | 109.5(2) |
| C(90)-C(91)-H(91B) | 109.5(2) |
| H(91A)-C(91)-H(91B) | 109.5 |
| C(90)-C(91)-H(91C) | 109.5(2) |
| H(91A)-C(91)-H(91C) | 109.5 |
| H(91B)-C(91)-H(91C) | 109.5 |
| C(90)-C(92)-H(92A) | 109.5(2) |
| C(90)-C(92)-H(92B) | 109.47(14) |
| H(92A)-C(92)-H(92B) | 109.5 |
| C(90)-C(92)-H(92C) | 109.5(2) |
| H(92A)-C(92)-H(92C) | 109.5 |
| H(92B)-C(92)-H(92C) | 109.5 |

Symmetry transformations used to generate equivalent atoms:

X(1A) is the centroid of C1 C2 C3 C4 and C5.

X(1B) is the centroid of C6 C7 C8 C9 and C10.

Pln(A) is the plane formed by C1 C2 C3 C4 and C5.

Pln(B) is the plane formed by C6 C7 C8 C9 and C10.

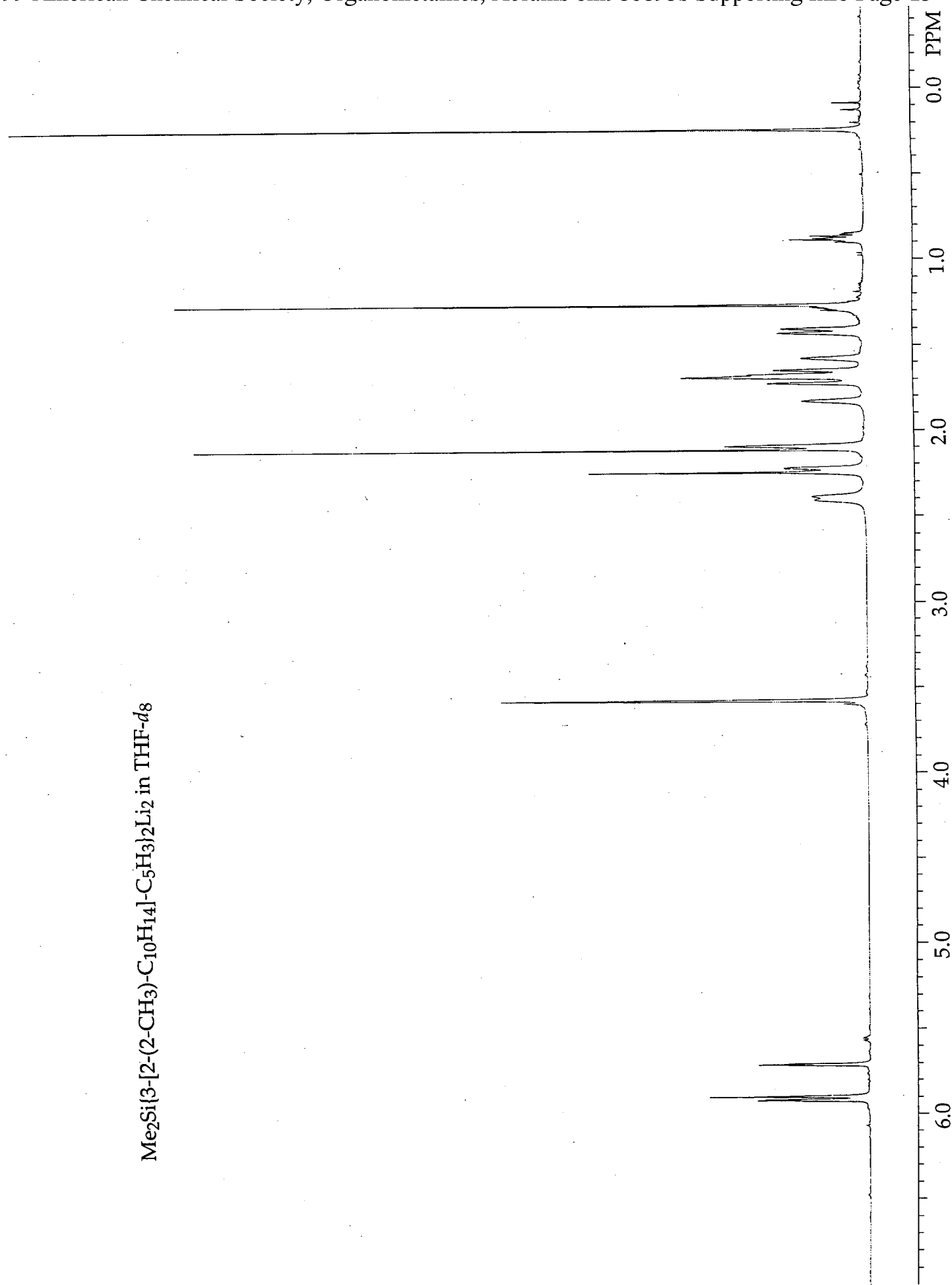
Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|--------|--------|--------|--------|-------|--------|---------|
| Sc | 20(1) | 26(1) | 25(1) | 0(1) | 4(1) | 1(1) |
| Si | 31(1) | 61(1) | 25(1) | 18(1) | 12(1) | 21(1) |
| C(1) | 20(1) | 43(2) | 20(1) | 4(1) | 3(1) | -4(1) |
| C(2) | 24(1) | 31(1) | 20(1) | 0(1) | 3(1) | -2(1) |
| C(3) | 32(1) | 26(1) | 34(1) | 2(1) | 13(1) | -3(1) |
| C(4) | 57(2) | 26(1) | 32(2) | -9(1) | 24(1) | -11(1) |
| C(5) | 39(2) | 41(2) | 20(1) | -2(1) | 5(1) | -17(1) |
| C(6) | 48(2) | 29(1) | 21(1) | 4(1) | 10(1) | 16(1) |
| C(7) | 63(2) | 24(1) | 19(1) | -2(1) | 4(1) | -5(1) |
| C(8) | 55(2) | 30(2) | 26(1) | 0(1) | -8(1) | -12(1) |
| C(9) | 43(2) | 26(1) | 23(1) | 4(1) | 1(1) | 3(1) |
| C(10) | 38(2) | 36(2) | 22(1) | 6(1) | 6(1) | 12(1) |
| C(11) | 41(2) | 132(4) | 50(2) | 50(2) | 14(2) | 38(3) |
| C(12) | 54(2) | 77(2) | 40(2) | 24(2) | 26(2) | 36(2) |
| C(13) | 48(2) | 54(2) | 74(3) | 4(2) | 38(2) | 3(2) |
| C(14A) | 35(3) | 48(7) | 122(7) | 25(4) | 48(4) | 15(3) |
| C(14B) | 19(4) | 39(9) | 104(9) | 13(6) | 27(5) | 1(4) |
| C(15) | 27(2) | 57(2) | 106(3) | 38(3) | 5(2) | 7(2) |
| C(30) | 41(2) | 38(2) | 65(2) | 19(2) | 30(2) | 13(1) |
| C(31) | 65(2) | 38(2) | 104(3) | 22(2) | 44(2) | 16(2) |
| C(32) | 53(2) | 72(3) | 60(2) | 33(2) | 8(2) | 24(2) |
| C(50) | 62(2) | 72(2) | 20(1) | 0(2) | -5(1) | -33(2) |
| C(51) | 143(5) | 256(8) | 47(3) | 48(3) | -48(3) | -145(5) |
| C(52) | 149(5) | 82(3) | 19(2) | -1(2) | 8(2) | 5(3) |
| C(70) | 93(3) | 32(2) | 18(1) | 0(1) | 0(2) | -18(2) |
| C(71) | 280(8) | 38(2) | 25(2) | -6(2) | 43(3) | -3(3) |
| C(72) | 113(3) | 123(4) | 28(2) | 19(2) | -23(2) | -59(3) |
| C(90) | 41(2) | 35(2) | 29(1) | 6(1) | 6(1) | 2(1) |
| C(91) | 101(3) | 47(2) | 42(2) | 7(2) | 21(2) | -18(2) |
| C(92) | 51(2) | 67(2) | 27(2) | 10(2) | 12(1) | -3(2) |

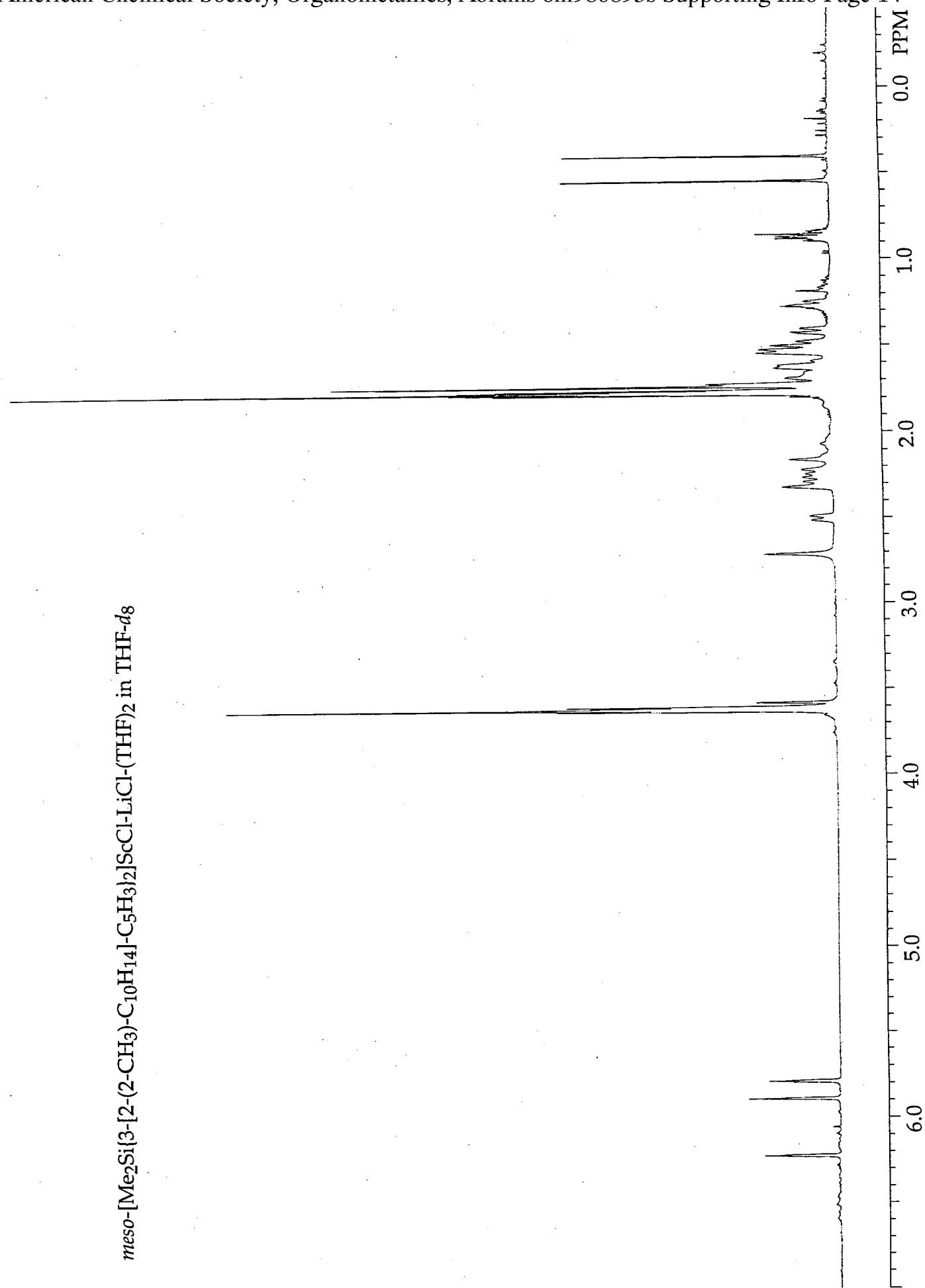
Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for δ .

| | x | y | z | U(eq) |
|--------|-----------|-----------|-----------|----------|
| H(11A) | 10064(7) | -32(21) | 9179(9) | 70(10) |
| H(11B) | 10824(12) | 636(14) | 8784(9) | 101(16) |
| H(11C) | 10569(12) | -674(17) | 8585(7) | 99(15) |
| H(12A) | 9438(8) | 865(18) | 6745(6) | 61(10) |
| H(12B) | 10237(13) | -85(14) | 7027(5) | 67(10) |
| H(12C) | 10413(12) | 1354(15) | 7119(4) | 98(15) |
| H(13A) | 6203 | 2305 | 9834 | 103(25) |
| H(13B) | 5588 | 1089 | 9562 | 106(23) |
| H(14A) | 5797 | 3267 | 8914 | 64(19) |
| H(15B) | 5270 | 2418 | 7676 | 64(17) |
| H(15A) | 5207 | 1124 | 8011 | 53(15) |
| H(13C) | 5913 | 2657 | 9588 | 230(83) |
| H(13D) | 5968 | 1195 | 9815 | 85(34) |
| H(14B) | 5197 | 772 | 8835 | 24(20) |
| H(15C) | 5458 | 2833 | 8037 | 10(15) |
| H(15D) | 5115 | 1529 | 7713 | 565(234) |
| H(31A) | 7861(12) | 5849(5) | 7220(9) | 76(11) |
| H(31B) | 7542(12) | 6115(8) | 8051(8) | 48(10) |
| H(31C) | 6809(9) | 6462(10) | 7356(10) | 75(10) |
| H(32A) | 6296(13) | 3260(15) | 6819(2) | 83(12) |
| H(32B) | 7160(9) | 4072(17) | 6507(6) | 67(10) |
| H(32C) | 6104(13) | 4676(13) | 6565(6) | 71(10) |
| H(51A) | 10328(10) | 2798(21) | 10283(11) | 112(13) |
| H(51B) | 9960(4) | 4003(18) | 9726(13) | 148(21) |
| H(51C) | 10433(10) | 2687(18) | 9359(11) | 77(12) |
| H(52A) | 8290(14) | 3743(17) | 10310(8) | 111(16) |
| H(52B) | 8689(10) | 2604(19) | 10776(9) | 67(10) |
| H(52C) | 7752(13) | 2450(18) | 10259(7) | 131(21) |
| H(71A) | 7547(14) | -1981(18) | 6459(13) | 102(15) |
| H(71B) | 8492(16) | -1387(16) | 6632(11) | 186(32) |
| H(71C) | 7960(18) | -1118(12) | 5931(13) | 83(11) |
| H(72A) | 5989(8) | -699(14) | 6493(10) | 128(17) |
| H(72B) | 6419(3) | 194(19) | 5911(9) | 91(12) |
| H(72C) | 6079(8) | 735(16) | 6655(8) | 34(9) |
| H(91A) | 6749(10) | -3315(8) | 9259(10) | 88(14) |
| H(91B) | 5817(13) | -3011(4) | 8763(9) | 65(10) |
| H(91C) | 5737(13) | -3214(7) | 9610(8) | 62(9) |
| H(92A) | 7404(10) | -1730(13) | 10184(3) | 57(9) |
| H(92B) | 6340(8) | -1585(14) | 10513(5) | 43(7) |
| H(92C) | 6896(11) | -367(13) | 10215(4) | 47(8) |
| H(2) | 8197(16) | 2572(21) | 7164(13) | 31(7) |
| H(4) | 7504(19) | 4090(24) | 9087(15) | 44(8) |
| H(8) | 5976(19) | -882(25) | 7811(15) | 48(8) |
| H(10) | 8308(17) | -648(23) | 9252(14) | 38(7) |
| H(30) | 6254(18) | 4616(22) | 7841(14) | 40(7) |
| H(50) | 9126(19) | 1554(25) | 9749(14) | 42(8) |
| H(70) | 7770(16) | 568(21) | 6675(12) | 23(6) |
| H(90) | 5716(19) | -1075(23) | 9356(14) | 37(8) |

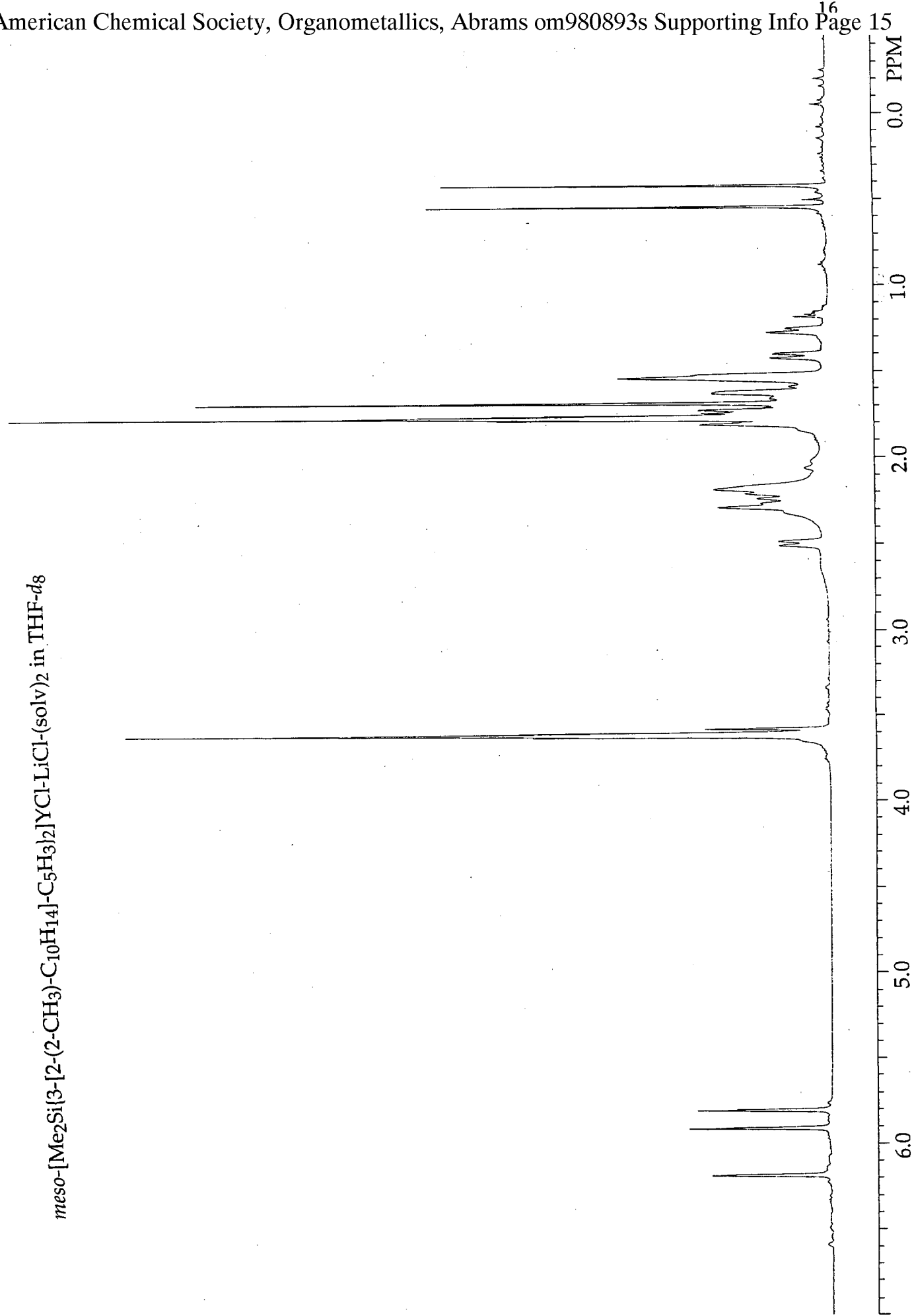
$\text{Me}_2\text{Si}\{\text{3-[2-(2-CH}_3\text{)-C}_{10}\text{H}_{14}\text{]-C}_5\text{H}_3\}_2\text{Li}_2$ in THF-*d*₈



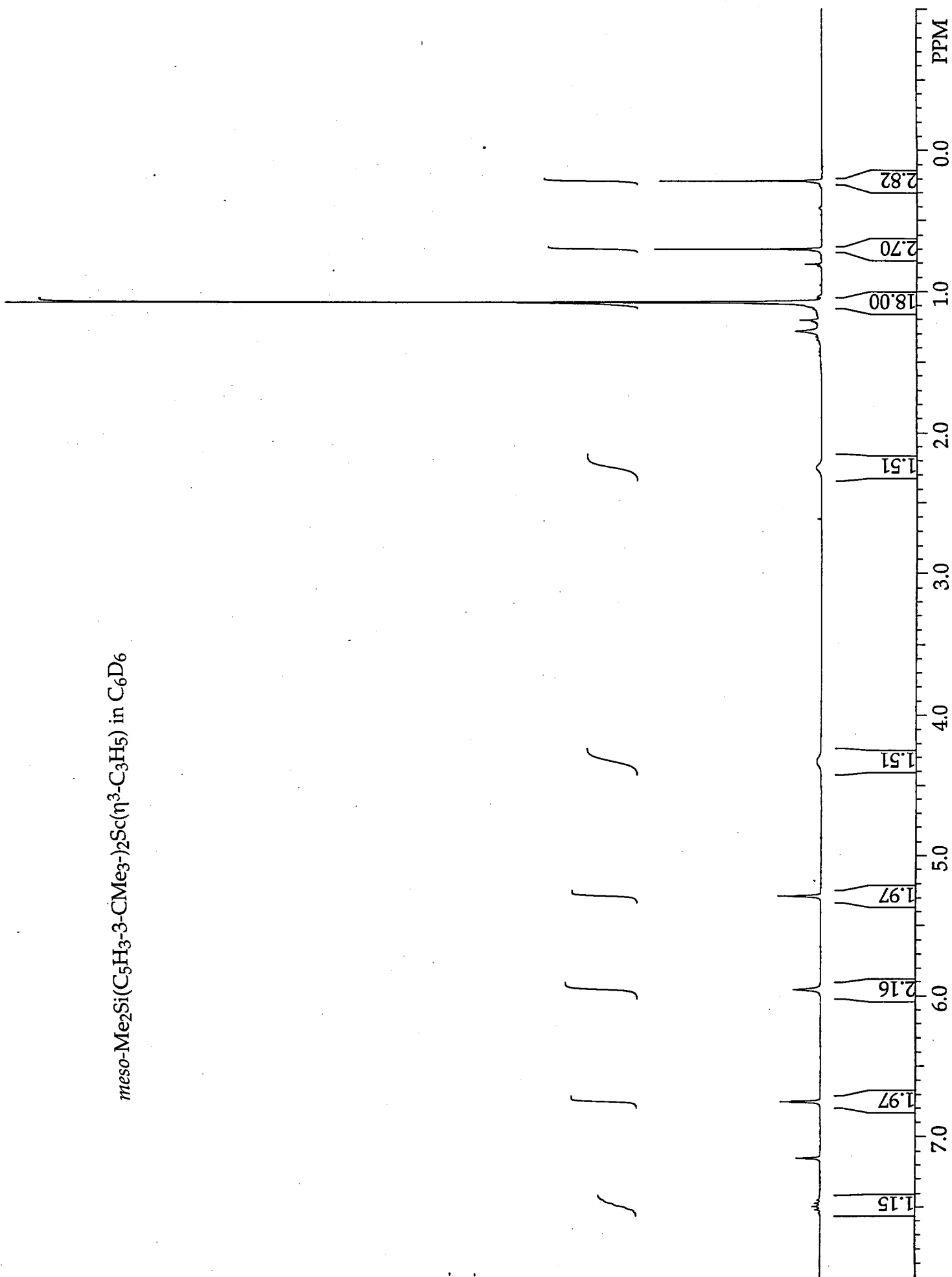
meso-[Me₂Si{3-[2-(2-CH₃)-C₁₀H₁₄]-C₅H₉]₂ScCl-LiCl-(THF)₂] in THF-*d*₈



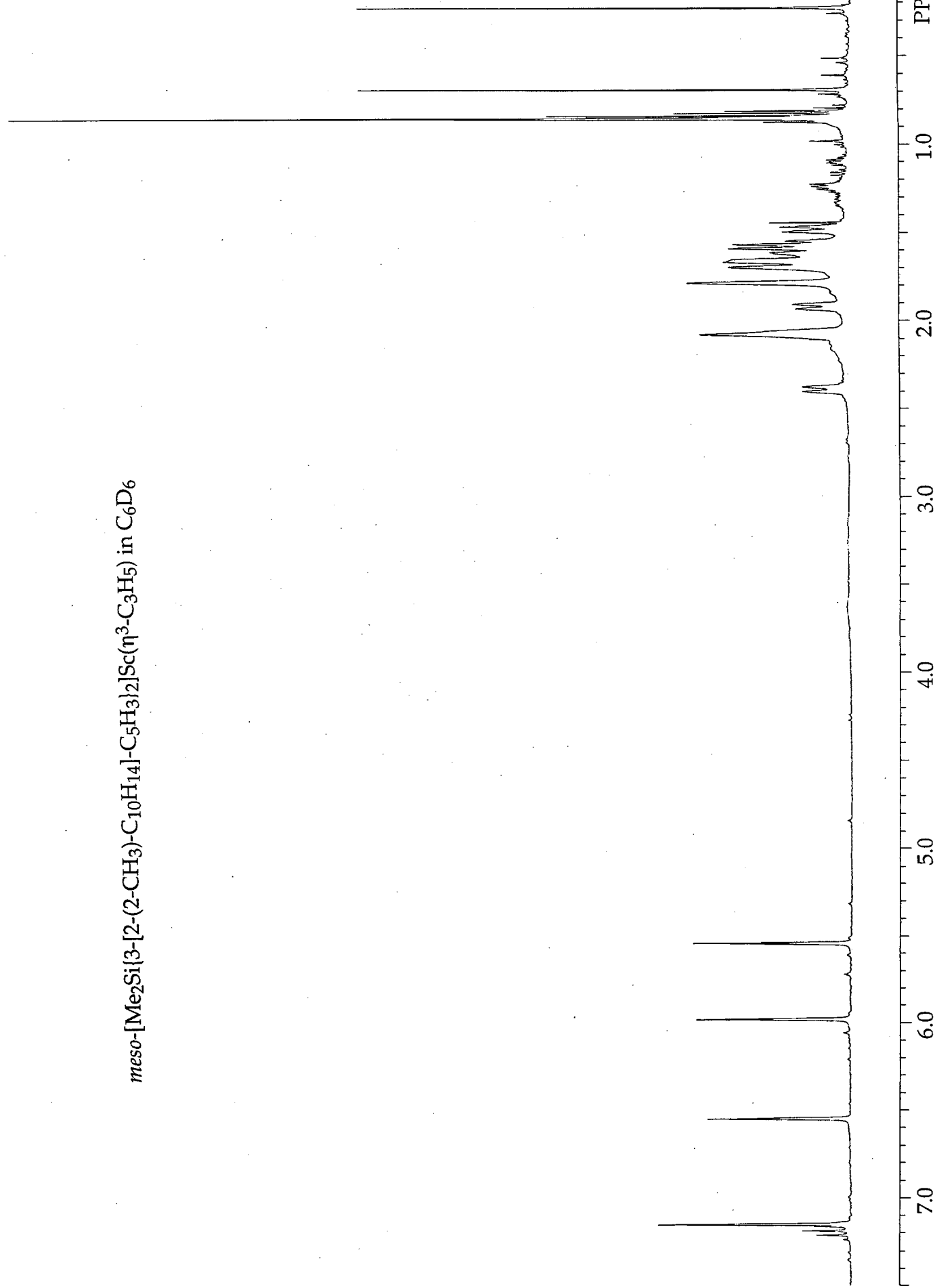
meso-[Me₂Si{3-[2-(2-CH₃)-C₁₀H₁₄]-C₅H₃]₂YCl-LiCl-(solv)₂] in THF-*d*₈



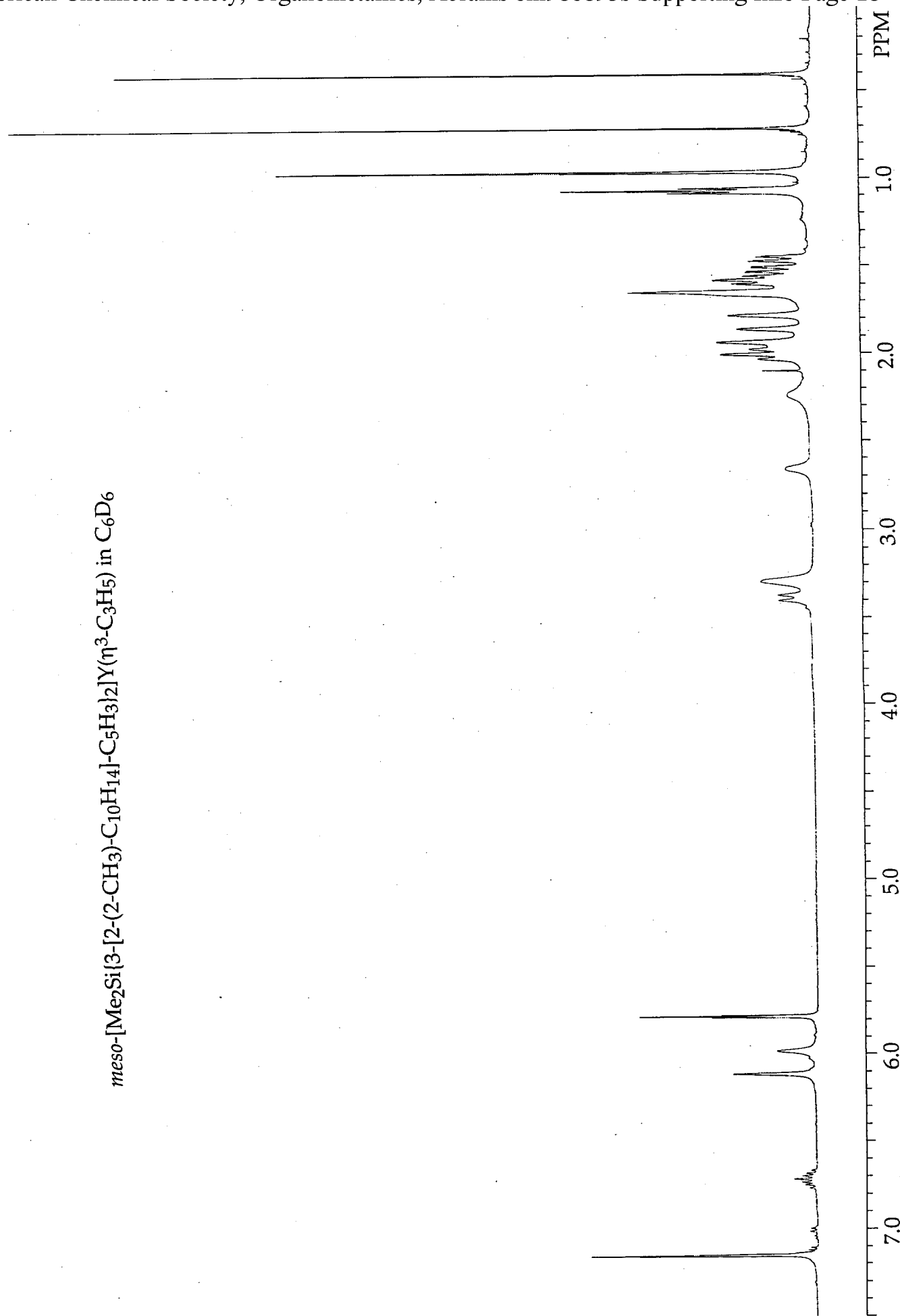
meso-Me₂Si(C₅H₃-3-CMe₃)₂Sc(η³-C₃H₅) in C₆D₆



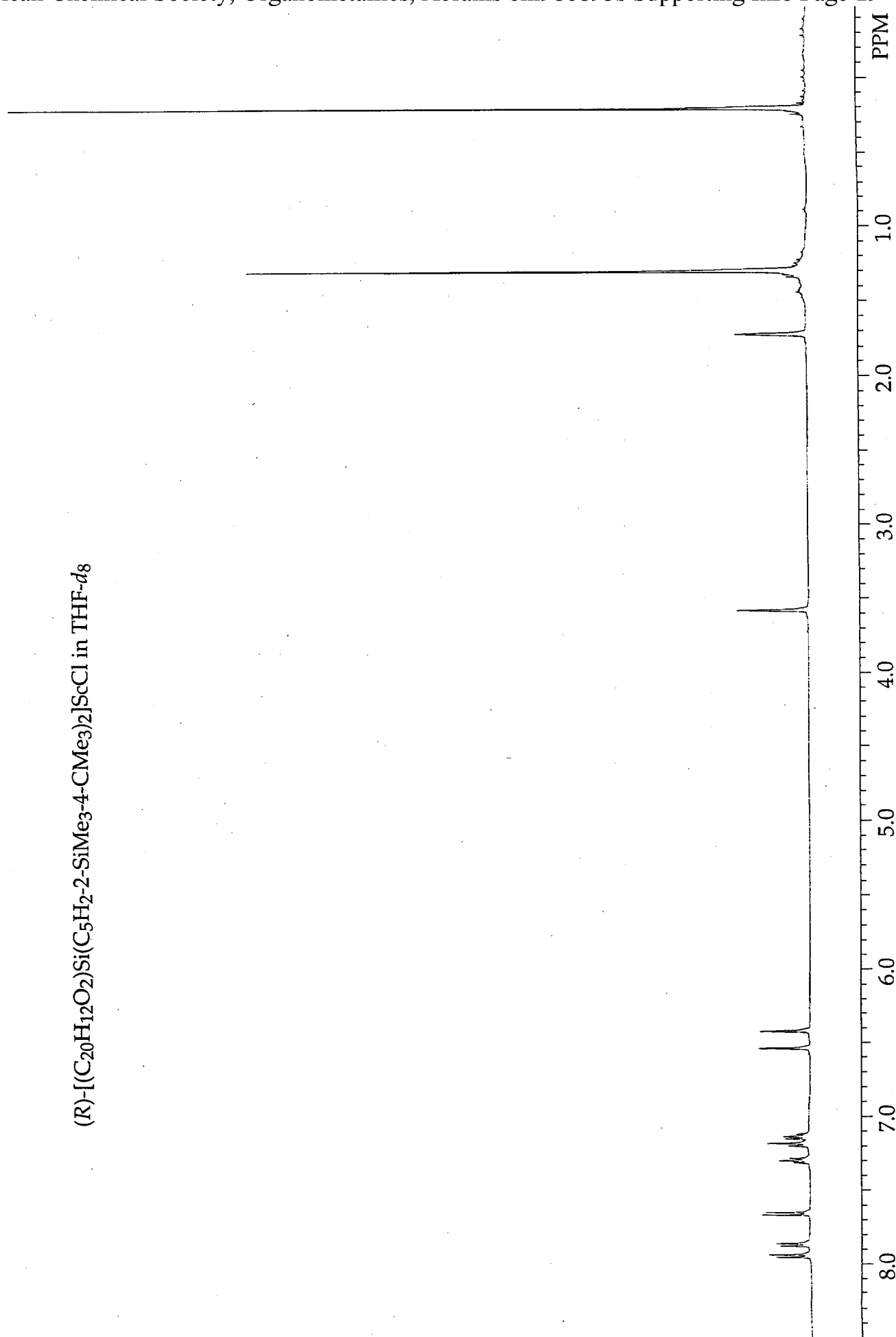
meso-[Me₂Si(3-[2-(2-CH₃)-C₁₀H₁₄]-C₅H₃)₂]Sc(η³-C₃H₅) in C₆D₆



meso-[Me₂Si(3-[2-(2-CH₃)-C₁₀H₁₄]-C₅H₃)₂Y(η³-C₃H₅)] in C₆D₆



(R)-[(C₂₀H₁₂O₂)Si(C₅H₂-2-SiMe₃-4-CMe₃)₂]ScCl in THF-d₈



(R)-[(C₂₀H₁₂O₂)Si(C₅H₂-2-SiMe₃-4-CMe₃)₂]Sc(η³-C₃H₅) in toluene-d₈

